

1-Chloro-1-nitropropane  
600-25-9 | DTXSID2024797

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 4.69e-02 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 7.87e-01

**Confidence level:** 7.88e-01

## Nearest Neighbors from the Training Set

Image not found

1-Chloro-1-nitropropane

**Measured:** 6.48e-02

**Predicted:** 4.69e-02

Image not found

1-Chloro-2-nitropropane

**Measured:** 6.48e-02

**Predicted:** 3.89e-02

Image not found

1,1-Dichloro-1-nitroethane

**Measured:** 1.74e-02

**Predicted:** 2.48e-02

Image not found

Propane, 1,1-dichloro-1-nitro-

**Measured:** 3.17e-02

**Predicted:** 3.17e-02